

Supplementary Table 1: Crystallographic and refinement statistics for native BPS1

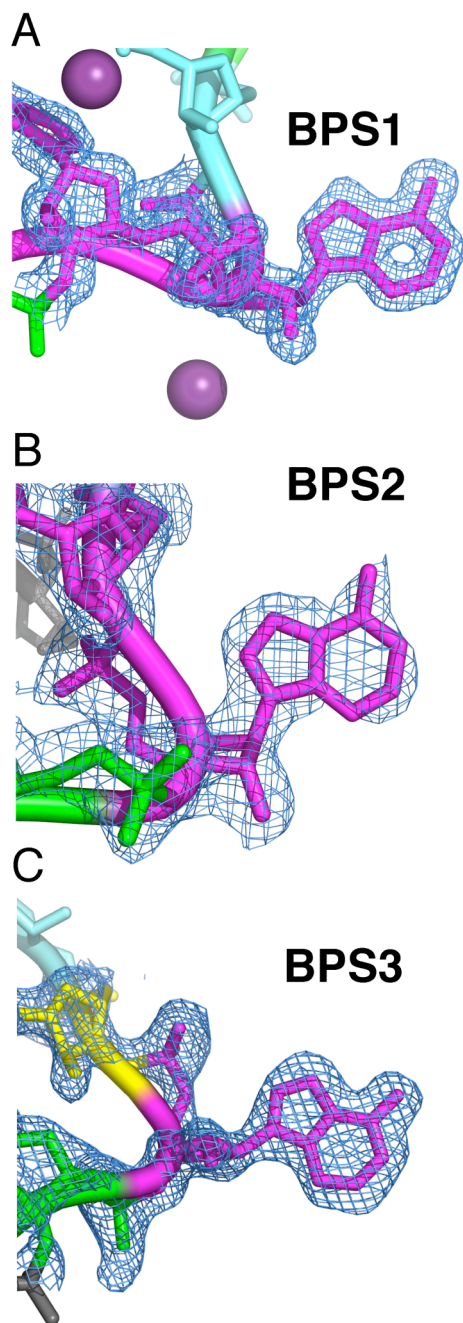
Sequence	BPS1 (native) 5'-G C G C G ψ A G U A G C G C G C <u>A</u> U C A U C G C - 5'
A: Data collection statistics	
Wavelength (Å)	1.54 Å
Space group	C2
Unit cell parameters	
a (Å)	68.70
b (Å)	41.01
c (Å)	32.97
β (°)	94.79
Resolution limit (Å)	2.55
Observed reflections	20,601
Unique reflections	3,027
Completeness ^a (%)	99.5 (100.0)
$I/\sigma(I)$ ^a	44.1 (16.5)
Redundancy ^a	6.8 (6.0)
$R_{\text{sym}}^{\text{a,b}}$ (%)	5.3 (10.8)
B: Refinement statistics	
$R_{\text{cryst}}^{\text{c}}$ (%)	19.3
$R_{\text{free}}^{\text{c}}$ (%)	22.7
RMSD bond lengths (Å)	0.005
RMSD bond angles (°)	0.96
Coordinate error from cross-validated Luzzati plot (Å)	
Coordinate error from cross-validated σ_A plot (Å)	
No. RNA atoms	528
No. water atoms	49
No. sulfate ions	1
No. iodide ions	0
No. magnesium ions	0
Average B-factor	
all atoms (Å ²)	15.1
RNA atoms (Å ²)	14.6
Water atoms (Å ²)	17.4

^a Values in parenthesis are for the highest resolution shell: 2.64-2.55 Å for BPS1

^b $R_{\text{merge}} = \sum_{hkl} \sum_i |I_i - \langle I \rangle| / \sum_{hkl} \sum_i I_i$, where I_i is an intensity I for the i th measurement of a reflection with indices hkl and $\langle I \rangle$ is the weighted mean of all measurements of I .

^c $R_{\text{cryst}} = \sum_{hkl} \sum_i |F_o(hkl) - k|F_c(hkl)| / \sum_{hkl} |F_o(hkl)|$ for the working set of reflections; R_{free} is R_{cryst} for 7% of the reflections excluded from the refinement

SUPPLEMENTARY FIGURE 1. Composite omit $2|F_o|-|F_c|$ electron density maps shown at 1σ contour level for the bulged adenosines of (A) BPS1, (B) BPS2, and (C) BPS3.



SUPPLEMENTARY FIGURE 2. Sulfate ions bound to junction of symmetry-related duplexes (distinguished by cyan and yellow coloring). An $|F_o|-|F_c|$ omit electron density map for the sulfates is shown at 3σ contour level. (A) BPS1. (B) BPS2.

